

\$%^STN;HighlightOn= \*\*\*;HighlightOff=\*\*\* i

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NEWS 24 JUL 28 IFICDB, IFIPAT, and IFIUDB reloaded with enhancements  
NEWS 25 JUL 28 STN Viewer performance improved

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STRUCTURE FILE UPDATES: 28 JUL 2008 HIGHEST RN 1036756-19-0  
DICTIONARY FILE UPDATES: 28 JUL 2008 HIGHEST RN 1036756-19-0

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=> Uploading C:\Program Files\STNEXP\Queries\10535043.str

## 1.1 STRUCTURE UPLOADED

=> d 11

L1 STR  
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*  
Structure attributes must be viewed using STN Express query preparation.

=> s 11  
SAMPLE SEARCH INITIATED 06:49:49 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 7 TO ITERATE  
100.0% PROCESSED 7 ITERATIONS 2 ANSWERS  
SEARCH TIME: 00.00.01  
FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 7 TO 298  
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s 11 sss full  
FULL SEARCH INITIATED 06:50:15 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 134 TO ITERATE

100.0% PROCESSED 134 ITERATIONS 10 ANSWERS  
SEARCH TIME: 00.00.01

L3 10 SEA SSS FUL L1

=> d scan

L3 10 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN  
IN 2-Propenoic acid, 3-[3-[(2-(acetoxy)-4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl)methyl](cyclohexylcarbonyl)amino]phenyl-, methyl ester  
MF C33 H39 N O7

/ Structure 1 in file .gra /

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 10 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN  
IN 2-Propenoic acid, 3-[3-[(4-(3-butoxy-3-oxo-1-propen-1-yl)-2-(2-ethoxy-2-oxoethoxy)phenyl)methyl](cyclohexylcarbonyl)aminolphenyl]-, methyl ester  
MF C35 H43 N O8

/ Structure 2 in file .gra /

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file cap  
 COST IN U.S. DOLLARS  
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FILE 'CAPLUS' ENTERED AT 06:51:03 ON 29 JUL 2008  
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FILE COVERS 1907 - 29 Jul 2008 VOL 149 ISS 5  
FILE LAST UPDATED: 28 Jul 2008 (20080728/ED)

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=> s 13  
L4 1 L3

⇒ `dbib abs bitstr`

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2007382121 CAPLUS <>LOGINID:20080729>>  
DOCUMENT NUMBER: 147:22696  
TITLE: 3D-QSAR studies with the aid of molecular docking for  
a series of non-steroidal FXR agonists  
AUTHOR(S): Zhang, Tao; Zhou, Jun-Hong; Shi, Liang-Wei; Zhu,  
Rui-Xin; Chen, Min-Bo  
CORPORATE SOURCE: Shanghai Institute of Organic Chemistry, Chinese  
Academy of Sciences, Shanghai, 200032, Peop. Rep.  
China  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2007),  
17(8), 2156-2160  
CODEN: BMCLB8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The farnesoid x receptor (FXR) has become a potential drug target for treating cholesterol-related and bile acid-related diseases recently. In this paper, 3-dimensional quant. structure-activity (structure-affinity and structure-efficacy) relationships are investigated for a series of nonsteroidal agonists (fexaramine series) by using the comparative mol. field anal. (Co-MFA), where mol. docking method (FlexX) is employed to construct mol. superimposition maps. A proposal to design some new agonists is discussed lastly.

IT      \*\*\*938197-65-0\*\*\*      \*\*\*938197-67-2\*\*\*      \*\*\*938197-86-5\*\*\*  
      \*\*\*938197-97-8\*\*\*      \*\*\*938197-98-9\*\*\*      \*\*\*938197-99-0\*\*\*  
      \*\*\*938198-00-6\*\*\*      \*\*\*938198-01-7\*\*\*      \*\*\*938198-02-8\*\*\*  
      \*\*\*938198-03-9\*\*\*

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(mol. docking and 3D-QSAR for a series of non-steroidal FXR agonists)

RN 938197-65-0 CAPLUS

CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 3 in file .gra /

RN 938197-67-2 CAPLUS

CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl](2-naphthalenylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 4 in file .gra /

RN 938197-86-5 CAPLUS

CN 2-Propenoic acid, 3-[3-[[benzoyl][4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 5 in file .gra /

RN 938197-97-8 CAPLUS

CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)-2-hydroxyphenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 6 in file .gra /

RN 938197-98-9 CAPLUS

CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)-2-methoxyphenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 7 in file .gra /

RN 938197-99-0 CAPLUS

CN 2-Propenoic acid, 3-[3-[[4-(3-butoxy-3-oxo-1-propen-1-yl)-2-(phenylmethoxy)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 8 in file .gra /

RN 938198-00-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[2-(acetyloxy)-4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 9 in file .gra /

RN 938198-01-7 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[2-(benzoyloxy)-4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 10 in file .gra /

RN 938198-02-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[4-(3-butoxy-3-oxo-1-propen-1-yl)-2-(methylsulfonyloxy)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 11 in file .gra /

RN 938198-03-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[4-(3-butoxy-3-oxo-1-propen-1-yl)-2-(2-ethoxy-2-oxoethoxy)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 12 in file .gra /

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file logoff  
'LOGOFF' IS NOT A VALID FILE NAME  
SESSION CONTINUES IN FILE 'CAPLUS'.  
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that are available. If you have requested multiple files, you can  
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accessing the remaining file names entered.

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.37	186.86
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL

	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.80	-0.80

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.12	186.98
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-0.80

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STRUCTURE FILE UPDATES: 28 JUL 2008 HIGHEST RN 1036756-19-0  
DICTIONARY FILE UPDATES: 28 JUL 2008 HIGHEST RN 1036756-19-0

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=>  
Uploading C:\Program Files\STNEXP\Queries\10535043 take 2.str

L5 STRUCTURE UPLOADED

=> d 15  
L5 HAS NO ANSWERS  
L5 STR

/ Structure 13 in file .gra /

Structure attributes must be viewed using STN Express query preparation.

=> s 15 sss sam  
SAMPLE SEARCH INITIATED 06:55:22 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 123 TO ITERATE

100.0% PROCESSED 123 ITERATIONS 3 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 1795 TO 3125  
PROJECTED ANSWERS: 3 TO 162

L6 3 SEA SSS SAM L5

=> s 15 sss ful  
FULL SEARCH INITIATED 06:55:31 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 2524 TO ITERATE

100.0% PROCESSED 2524 ITERATIONS 90 ANSWERS  
SEARCH TIME: 00.00.01

L7 90 SEA SSS FUL L5

	SINCE FILE	TOTAL
	ENTRY	SESSION
COST IN U.S. DOLLARS		
FULL ESTIMATED COST	178.36	365.34
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-0.80

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FILE COVERS 1907 - 29 Jul 2008 VOL 149 ISS 5  
FILE LAST UPDATED: 28 Jul 2008 (20080728/ED)

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```
=> s 17
L8          13 L7

=> d 1-13 ibib abs hitstr
```

L8 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2007:382121 CAPLUS <<LOGINID:20080729>>  
DOCUMENT NUMBER: 147:22696  
TITLE: 3D-QSAR studies with the aid of molecular docking for  
a series of non-steroidal FXR agonists  
AUTHOR(S): Zhang, Tao; Zhou, Jun-Hong; Shi, Liang-Wei; Zhu,  
Rui-Xin; Chen, Min-Bo  
CORPORATE SOURCE: Shanghai Institute of Organic Chemistry, Chinese  
Academy of Sciences, Shanghai, 200032, Peop. Rep.  
China  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2007),  
17(8), 2156-2160  
CODEN: BMCLE8; ISSN: 0960-894X  
PUBLISHER: Elsevier Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The farnesoid x receptor (FXR) has become a potential drug target for  
treating cholesterol-related and bile acid-related diseases recently. In  
this paper, 3-dimensional quant. structure-activity (structure-affinity  
and structure-efficacy) relationships are investigated for a series of  
nonsteroidal agonists (fexaramine series) by using the comparative mol.  
field anal. (Co-MFA), where mol. docking method (FlexX) is employed to  
construct mol. superimposition maps. A proposal to design some new  
agonists is discussed lastly.

IT \*\*\*\*574013-66-4\*\*\* \*\*\*\*574013-67-5\*\*\* \*\*\*\*574013-68-6\*\*\*  
\*\*\*\*592525-03-6\*\*\* \*\*\*\*592525-04-7\*\*\* \*\*\*\*592525-05-8\*\*\*  
\*\*\*\*592525-07-0\*\*\* \*\*\*\*592525-08-1\*\*\* \*\*\*\*592525-09-2\*\*\*  
\*\*\*\*592525-10-5\*\*\* \*\*\*\*592525-21-8\*\*\* \*\*\*\*592525-25-2\*\*\*  
\*\*\*\*592525-26-3\*\*\* \*\*\*\*592525-27-4\*\*\* \*\*\*\*592525-28-5\*\*\*  
\*\*\*\*592525-29-6\*\*\* \*\*\*\*592525-32-1\*\*\* \*\*\*\*592525-35-4\*\*\*  
\*\*\*\*592525-38-7\*\*\* \*\*\*\*592525-41-2\*\*\* \*\*\*\*592525-44-5\*\*\*  
\*\*\*\*592525-47-8\*\*\* \*\*\*\*592525-50-3\*\*\* \*\*\*\*592525-55-8\*\*\*  
\*\*\*\*592525-58-1\*\*\* \*\*\*\*592525-61-6\*\*\* \*\*\*\*592525-64-9\*\*\*  
\*\*\*\*592525-67-2\*\*\* \*\*\*\*592525-72-9\*\*\* \*\*\*\*592525-78-5\*\*\*  
\*\*\*\*592525-81-0\*\*\* \*\*\*\*592525-84-3\*\*\* \*\*\*\*592525-87-6\*\*\*  
\*\*\*\*592525-90-1\*\*\* \*\*\*\*592525-93-4\*\*\* \*\*\*\*592525-98-9\*\*\*  
\*\*\*\*592526-01-7\*\*\* \*\*\*\*592526-04-0\*\*\* \*\*\*\*592526-07-3\*\*\*  
\*\*\*\*592526-12-0\*\*\* \*\*\*\*938197-64-9\*\*\* \*\*\*\*938197-65-0\*\*\*  
\*\*\*\*938197-67-2\*\*\* \*\*\*\*938197-74-1\*\*\* \*\*\*\*938197-75-2\*\*\*  
\*\*\*\*938197-76-3\*\*\* \*\*\*\*938197-77-4\*\*\* \*\*\*\*938197-78-5\*\*\*  
\*\*\*\*938197-79-6\*\*\* \*\*\*\*938197-80-9\*\*\* \*\*\*\*938197-81-0\*\*\*  
\*\*\*\*938197-82-1\*\*\* \*\*\*\*938197-86-5\*\*\* \*\*\*\*938197-92-3\*\*\*  
\*\*\*\*938197-93-4\*\*\* \*\*\*\*938197-95-6\*\*\* \*\*\*\*938197-96-7\*\*\*  
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic  
use); BIOL (Biological study); USES (Uses)  
(mol. docking and 3D-QSAR for a series of non-steroidal FXR agonists)  
RN 574013-66-4 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 14 in file .gra /

RN 574013-67-5 CAPLUS

CN 2-Propenoic acid, 3-[3-[[[4-(1,3-benzodioxol-5-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 15 in file .gra /

RN 574013-68-6 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(2-phenylethenyl)phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 16 in file .gra /

RN 592525-03-6 CAPLUS

CN 2-Propenoic acid, 3-[3-[[[4-(2-carboxyethenyl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, 1-methyl ester (CA INDEX NAME)

/ Structure 17 in file .gra /

RN 592525-04-7 CAPLUS

CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 18 in file .gra /

RN 592525-05-8 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(3-ethoxy-3-oxo-1-propen-1-yl)phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 19 in file .gra /

RN 592525-07-0 CAPLUS

CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, phenylmethyl ester (CA INDEX NAME)

/ Structure 20 in file .gra /

RN 592525-08-1 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[3-(dimethylamino)-3-oxo-1-propen-1-yl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 21 in file .gra /

RN 592525-09-2 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-methoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 22 in file .gra /

RN 592525-10-5 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-ethoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 23 in file .gra /

RN 592525-21-8 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 24 in file .gra /

RN 592525-25-2 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(5-methyl-2-thienyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 25 in file .gra /

RN 592525-26-3 CAPLUS

CN 2-Propenoic acid, 3-[3-[[[4-(5-acetyl-2-thienyl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 26 in file .gra /

RN 592525-27-4 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methoxyphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 27 in file .gra /

RN 592525-28-5 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-[4-(1,1-dimethylethyl)phenyl]ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 28 in file .gra /

RN 592525-29-6 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methylphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 29 in file .gra /

RN 592525-32-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2,6-dichlorophenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 30 in file .gra /

RN 592525-35-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[[4-[2-(3-chlorophenyl)ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 31 in file .gra /

RN 592525-38-7 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[[4-[2-[3,5-bis(trifluoromethyl)phenyl]ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 32 in file .gra /

RN 592525-41-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-[3-(trifluoromethyl)phenyl]ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 33 in file .gra /

RN 592525-44-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2,6-difluorophenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 34 in file .gra /

RN 592525-47-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2-fluorophenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 35 in file .gra /

RN 592525-50-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2,4,6-trimethylphenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 36 in file .gra /

RN 592525-55-8 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(3-fluorophenyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 37 in file .gra /

RN 592525-58-1 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(4-fluorophenyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 38 in file .gra /

RN 592525-61-6 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(2-pyridinyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 39 in file .gra /

RN 592525-64-9 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(4-methyl-5-thiazolyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 40 in file .gra /

RN 592525-67-2 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',4'-difluoro[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 41 in file .gra /

RN 592525-72-9 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 42 in file .gra /

RN 592525-78-5 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-ethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 43 in file .gra /

RN 592525-81-0 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 44 in file .gra /

RN 592525-84-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-chloro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 45 in file .gra /

RN 592525-87-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 46 in file .gra /

RN 592525-90-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 47 in file .gra /

RN 592525-93-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(5'-chloro-2'-methoxy[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 48 in file .gra /

RN 592525-98-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-chloro-4'-fluoro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 49 in file .gra /

RN 592526-01-7 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 50 in file .gra /

RN 592526-04-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 51 in file .gra /

RN 592526-07-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2',6'-dimethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 52 in file .gra /

RN 592526-12-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 53 in file .gra /

RN 938197-64-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(5-cyclohexyl-2-thienyl)phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 54 in file .gra /

RN 938197-65-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 55 in file .gra /

RN 938197-67-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl](2-naphthalenylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 56 in file .gra /

RN 938197-74-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(4-methylthio)phenyl]ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 57 in file .gra /

RN 938197-75-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(3-methoxyphenyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 58 in file .gra /

RN 938197-76-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[[4-[2-(3-acetylphenyl)ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 59 in file .gra /

RN 938197-77-4 CAPLUS

CN 2-Propenoic acid, 3-[3-[(4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, ethyl ester (CA INDEX NAME)

/ Structure 60 in file .gra /

RN 938197-78-5 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(3-butoxy-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]phenyl]-, butyl ester (CA INDEX NAME)

/ Structure 61 in file .gra /

RN 938197-79-6 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(3-amino-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]phenyl]-, butyl ester (CA INDEX NAME)

/ Structure 62 in file .gra /

RN 938197-80-9 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-methoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, butyl ester (CA INDEX NAME)

/ Structure 63 in file .gra /

RN 938197-81-0 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-ethoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, butyl ester (CA INDEX NAME)

/ Structure 64 in file .gra /

RN 938197-82-1 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-phenoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, butyl ester (CA INDEX NAME)

/ Structure 65 in file .gra /

RN 938197-86-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(benzoyl)[4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 66 in file .gra /

RN 938197-92-3 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, propyl ester (CA INDEX NAME)

/ Structure 67 in file .gra /

RN 938197-93-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-[3-(butylamino)-3-oxo-1-propen-1-yl]phenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 68 in file .gra /

RN 938197-95-6 CAPLUS  
CN Benzenepropanoic acid, 4-[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]-, butyl ester (CA INDEX NAME)

/ Structure 69 in file .gra /

RN 938197-96-7 CAPLUS  
CN Benzenepropanoic acid, 4-[[3-(3-butoxy-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]-, butyl ester (CA INDEX NAME)

/ Structure 70 in file .gra /

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2007:331294 CAPLUS <>LOGINID::20080729>>  
DOCUMENT NUMBER: 148:419  
TITLE: Comparative studies of prediction of herb-based FXR  
ligands by 11 binding free energies scoring functions  
AUTHOR(S): Wei, Zhu; Qin, Huang; Li, Xudong; Chen, Keji; Xu,  
Xiaojie

CORPORATE SOURCE: Guangdong Hospital of Traditional Chinese Medicine,  
Guangzhou, 510106, Peop. Rep. China

SOURCE: Jisuanji Yu Yingyong Huaxue (2007), 24(1), 94-96  
CODEN: JYYHE6; ISSN: 1001-4160

PUBLISHER: Jisuanji Yu Yingyong Huaxue Bianjibu

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB Based on the optimized complex structure of FXR bound with specific  
ligand-fexaramine (PDB code 1OSH), computer-aided structure-based virtual  
screening against Peking University Drug Design System (PKUDSS) was  
conducted to det. the occurrence of herb-based FXR ligands. 11 Scoring  
functions (igscore1, Ligscore2, D-Score, -PLP1, -PLP2, Jain, -PMF, Ludil,  
Ludi2, Ludi3 and consensus) have been compared to evaluate their  
prediction ability after conformational sampling by program Ligandfit.  
The results suggest that -PLP1 and -PLP2 have better prediction ability  
than others.

IT \*\*\*574013-66-4\*\*\* , Fexaramine

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
(Biological study); USES (Uses)  
(comparative studies of prediction of herb-based FXR ligands by 11  
binding free energies scoring functions)

RN 574013-66-4 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[4'-(dimethylamino)[1,1'-  
biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 71 in file .gra /

L8 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2007:157205 CAPLUS <<LOGINID:20080729>>  
DOCUMENT NUMBER: 146:434160  
TITLE: 3D QSAR comparative molecular field analysis on  
nonsteroidal farnesoid X receptor activators  
AUTHOR(S): Honorio, Kathia M.; Garratt, Richard C.; Polikarpov,  
Igor; Andricopulo, Adriano D.  
CORPORATE SOURCE: Laboratorio de Quimica Medicinal e Computacional,  
Centro de Biotecnologia Molecular Estrutural,  
Instituto de Fisica de Sao Carlos, Universidade de Sao  
Paulo, Sao Carlos, SP, 13560-970, Brazil  
SOURCE: Journal of Molecular Graphics & Modelling (2007),  
25(6), 921-927  
CODEN: JMGMF1; ISSN: 1093-3263  
PUBLISHER: Elsevier Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Three-dimensional quant. structure-activity relationships (3D QSAR) were  
performed for a series of farnesoid X receptor activators using  
comparative mol. field anal. (CoMFA). A training set contg. 77 compds.  
served to establish the models. The best statistical results among all  
models were obtained with region focusing weighted by a S.D. \*times.  
coeff. values of 0.8 and a grid spacing of 1.0 ( $r^2 = 0.963$ ,  $SEE = 0.097$ ;  
 $q^2 = 0.742$ ,  $SEP = 0.255$ ). The model was used to predict the potency of 20  
test set compds. that were not included in the training set, and the  
predicted values were in good agreement with the exptl. results. The  
final CoMFA model along with the information obtained from 3D contour maps  
should be useful for the design of novel FXR ligands having improved  
potency.  
IT      \*\*\*592524-79-3\*\*\*      \*\*\*592524-80-6\*\*\*      \*\*\*592524-91-9\*\*\*  
      \*\*\*592525-09-2\*\*\*      \*\*\*592525-32-1\*\*\*      \*\*\*592525-58-1\*\*\*  
      \*\*\*592525-81-0\*\*\*      \*\*\*592526-01-7\*\*\*      \*\*\*934543-51-8\*\*\*  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
(Biological study); USES (Uses)  
      (3D QSAR comparative mol. field anal. on nonsteroidal farnesoid X  
      receptor activators)  
RN 592524-79-3 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-methoxy-1-propen-1-  
yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 72 in file .gra /

RN 592524-80-6 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-ethoxy-1-propen-1-  
yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 73 in file .gra /

RN 592524-91-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)(phenylmethyl)amino]phenyl]-,

methyl ester (CA INDEX NAME)

/ Structure 74 in file .gra /

RN 592525-09-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][4-(3-methoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 75 in file .gra /

RN 592525-32-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][4-[2-(2,6-dichlorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 76 in file .gra /

RN 592525-58-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][4-[2-(4-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 77 in file .gra /

RN 592525-81-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][4'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 78 in file .gra /

RN 592526-01-7 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 79 in file .gra /

RN 934543-51-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[benzoyl][4-(5-methyl-2-thienyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 80 in file .gra /

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2006:383580 CAPLUS <>LOGINID::20080729>>  
DOCUMENT NUMBER: 144:404429  
TITLE: A method using farnesoid X receptor (FXR) agonists with PPAR agonists for reducing drug-induced adverse

INVENTOR(S): side effects in a patient  
 Fiorucci, Stefano; Pellicciari, Roberto; Pruzanski, Mark  
 PATENT ASSIGNEE(S): Intercept Pharmaceuticals Inc., USA  
 SOURCE: PCT Int. Appl., 35 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006044391	A1	20060427	WO 2005-US36536	20051014
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, NX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BE, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
US 20060252670	A1	20061109	US 2005-250298	20051013
AU 2005295888	A1	20060427	AU 2005-295888	20051014
CA 2584284	A1	20060427	CA 2005-2584284	20051014
EP 1814582	A1	20070808	EP 2005-807696	20051014
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
JP 2008516955	T	20080522	JP 2007-536810	20051014
PRIORITY APPN. INFO.:			US 2004-619381P	P 20041014
			WO 2005-US36536	W 20051014

AB The invention relates to the discovery that farnesoid X receptor (FXR) agonists can be used in combination with peroxisome proliferation activated receptor  $\gamma$ . (PPAR. $\gamma$ .) agonists to reduce drug-induced adverse side effects in patients suffering from conditions such as insulin resistance, Type II diabetes, metabolic syndrome, non-alc. fatty liver disease (NAFLD), non-alc. steatohepatitis (NASH), and heart disease. Particularly, the invention encompasses methods for treating patients suffering from drug-induced adverse side effects with selective PPAR. $\gamma$ ., dual PPAR $\alpha$ /. $\gamma$ . and pan PPAR $\alpha$ /. $\gamma$ ./.delta. agonists in combination with FXR agonists.

IT \*\*\*574013-66-4\*\*\* , Fexaramine  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (FXR agonist combination with PPAR agonist for redn. of drug-induced adverse effects)  
 RN 574013-66-4 CAPLUS  
 CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2005:1049799 CAPLUS <<LOGINID::20080729>>  
DOCUMENT NUMBER: 143:319188  
TITLE: Treatment of fibrosis using farnesoid X receptor (FXR)  
ligands  
INVENTOR(S): Fiorucci, Stefano; Pellicciari, Roberto; Pruzanski,  
Mark  
PATENT ASSIGNEE(S): Intercept Pharmaceuticals, Inc., USA  
SOURCE: PCT Int. Appl., 70 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005089316	A2	20050929	WO 2005-US8575	20050314
WO 2005089316	A3	20060406		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005222994	A1	20050929	AU 2005-222994	20050314
CA 2559476	A1	20050929	CA 2005-2559476	20050314
US 20060069070	A1	20060330	US 2005-81002	20050314
EP 1734970	A2	20061227	EP 2005-729394	20050314
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
JP 2007529427	T	20071025	JP 2007-503111	20050314
PRIORITY APPN. INFO.:			US 2004-552865P	P 20040312
			WO 2005-US8575	W 20050314

AB The invention discloses a method for inhibiting fibrosis that occurs in an organ where the farnesoid X receptor (FXR) is expressed. The method involves administering a high potency, activating ligand of FXR in an effective amt. to a patient who is not suffering from a cholestatic condition. The invention also provides pharmaceutical compns. contg. an effective amt. of an FXR ligand and kits for dispensing the pharmaceutical compns.

IT \*\*\*574013-66-4\*\*\* , Fexaramine  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
(Biological study); USES (Uses)  
(farnesoid X receptor ligands for treatment of fibrosis)  
RN 574013-66-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4'-(dimethylamino){1,1'-biphenyl]-4-yl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 82 in file .gra /

L8 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2005:511387 CAPLUS <>LOGINID:20080729>>  
DOCUMENT NUMBER: 143:125843  
TITLE: Hologram quantitative structure-activity relationships  
for a series of farnesoid X receptor activators  
AUTHOR(S): Honorio, Kathia M.; Garratt, Richard C.; Andricopulo,  
Adriano D.  
CORPORATE SOURCE: Instituto de Fisica de Sao Carlos, Centro de  
Biotecnologia Molecular Estrutural, Laboratorio de  
Quimica Medicinal e Computacional, Universidade de Sao  
Paulo, Sao Carlos-SP, 13560-970, Brazil  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005),  
15(12), 3119-3125  
CODEN: BMCL8; ISSN: 0960-894X  
PUBLISHER: Elsevier B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The farnesoid X receptor (FXR) is an attractive drug target for the development of novel therapeutic agents for the treatment of dyslipidemia and cholestasis. Hologram quant. structure-activity relationship (HQSAR) studies were conducted on a series of potent FXR activators originated from natural product-like libraries. A training set contg. 82 compds. served to establish the models. The best HQSAR model was generated using atoms, bonds, connections, chirality, and donor and acceptor as fragment distinction and fragment size default (4-7) with six components. The model was used to predict the potency of 20 test set compds. that were not included in the training set, and the predicted values were in good agreement with the exptl. results. The final HQSAR model and the information obtained from HQSAR 2D contribution maps should be useful for the design of novel FXR ligands having improved potency.

IT \*\*\*\*574013-66-4\*\*\*\* \*\*\*\*574013-67-5\*\*\*\* \*\*\*\*592524-78-2\*\*\*\*  
\*\*\*\*592524-79-3\*\*\*\* \*\*\*\*592524-80-6\*\*\*\* \*\*\*\*592524-85-1\*\*\*\*  
\*\*\*\*592524-91-9\*\*\*\* \*\*\*\*592524-95-3\*\*\*\* \*\*\*\*592524-96-4\*\*\*\*  
\*\*\*\*592525-03-6\*\*\*\* \*\*\*\*592525-04-7\*\*\*\* \*\*\*\*592525-05-8\*\*\*\*  
\*\*\*\*592525-07-0\*\*\*\* \*\*\*\*592525-08-1\*\*\*\* \*\*\*\*592525-09-2\*\*\*\*  
\*\*\*\*592525-10-5\*\*\*\* \*\*\*\*592525-13-8\*\*\*\* \*\*\*\*592525-21-8\*\*\*\*  
\*\*\*\*592525-22-9\*\*\*\* \*\*\*\*592525-23-0\*\*\*\* \*\*\*\*592525-25-2\*\*\*\*  
\*\*\*\*592525-26-3\*\*\*\* \*\*\*\*592525-27-4\*\*\*\* \*\*\*\*592525-32-1\*\*\*\*  
\*\*\*\*592525-35-4\*\*\*\* \*\*\*\*592525-38-7\*\*\*\* \*\*\*\*592525-47-8\*\*\*\*  
\*\*\*\*592525-55-8\*\*\*\* \*\*\*\*592525-58-1\*\*\*\* \*\*\*\*592525-61-6\*\*\*\*  
\*\*\*\*592525-64-9\*\*\*\* \*\*\*\*592525-67-2\*\*\*\* \*\*\*\*592525-78-5\*\*\*\*  
\*\*\*\*592525-81-0\*\*\*\* \*\*\*\*592525-84-3\*\*\*\* \*\*\*\*592525-90-1\*\*\*\*  
\*\*\*\*592525-93-4\*\*\*\* \*\*\*\*592525-98-9\*\*\*\* \*\*\*\*592526-01-7\*\*\*\*  
\*\*\*\*592526-04-0\*\*\*\* \*\*\*\*592526-07-3\*\*\*\* \*\*\*\*592526-12-0\*\*\*\*  
\*\*\*\*592526-15-3\*\*\*\*

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(hologram quant. structure-activity relationships for a series of farnesoid X receptor activators)

RN 574013-66-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 83 in file .gra /

RN 574013-67-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[4-(1,3-benzodioxol-5-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 84 in file .gra /

RN 592524-78-2 CAPLUS  
CN 2-Propenoic acid, 3-[4-[[3-(3-amino-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 85 in file .gra /

RN 592524-79-3 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-methoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 86 in file .gra /

RN 592524-80-6 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-ethoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 87 in file .gra /

RN 592524-85-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[benzoyl[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 88 in file .gra /

RN 592524-91-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)(phenylmethyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 89 in file .gra /

RN 592524-95-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-bromophenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 90 in file .gra /

RN 592524-96-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 91 in file .gra /

RN 592525-03-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-(2-carboxyethenyl)phenyl)methyl](cyclohexylcarbonyl)amino]phenyl-, 1-methyl ester (CA INDEX NAME)

/ Structure 92 in file .gra /

RN 592525-04-7 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 93 in file .gra /

RN 592525-05-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[4-(3-ethoxy-3-oxo-1-propen-1-yl)phenyl]methyl]amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 94 in file .gra /

RN 592525-07-0 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl-, phenylmethyl ester (CA INDEX NAME)

/ Structure 95 in file .gra /

RN 592525-08-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[4-[3-(dimethylamino)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 96 in file .gra /

RN 592525-09-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[4-(3-methoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 97 in file .gra /

RN 592525-10-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[4-(3-ethoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 98 in file .gra /

RN 592525-13-8 CAPLUS  
CN Benzenepropanoic acid, 4-[(cyclohexylcarbonyl)[3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]amino]methyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 99 in file .gra /

RN 592525-21-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)((3'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 100 in file .gra /

RN 592525-22-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-acetyl[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 101 in file .gra /

RN 592525-23-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-(methylthio)[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 102 in file .gra /

RN 592525-25-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-(5-methyl-2-thienyl)phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 103 in file .gra /

RN 592525-26-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-(5-acetyl-2-thienyl)phenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 104 in file .gra /

RN 592525-27-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(4-methoxyphenyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 105 in file .gra /

RN 592525-32-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(2,6-dichlorophenyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 106 in file .gra /

RN 592525-35-4 CAPLUS

CN 2-Propenoic acid, 3-[3-[(4-[2-(3-chlorophenyl)ethenyl]phenyl)methyl](cyclohexylcarbonyl)aminophenyl]-, methyl ester (CA INDEX NAME)

/ Structure 107 in file .gra /

RN 592525-38-7 CAPLUS

CN 2-Propenoic acid, 3-[3-[(4-[2-[3,5-bis(trifluoromethyl)phenyl]ethenyl]phenyl)methyl](cyclohexylcarbonyl)aminophenyl]-, methyl ester (CA INDEX NAME)

/ Structure 108 in file .gra /

RN 592525-47-8 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(2-fluorophenyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 109 in file .gra /

RN 592525-55-8 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(3-fluorophenyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 110 in file .gra /

RN 592525-58-1 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(4-fluorophenyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 111 in file .gra /

RN 592525-61-6 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(2-pyridinyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 112 in file .gra /

RN 592525-64-9 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(4-methyl-5-thiazolyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 113 in file .gra /

RN 592525-67-2 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',4'-difluoro[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 114 in file .gra /

RN 592525-78-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)((3'-ethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 115 in file .gra /

RN 592525-81-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)((4'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 116 in file .gra /

RN 592525-84-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-chloro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 117 in file .gra /

RN 592525-90-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)((3'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 118 in file .gra /

RN 592525-93-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(5'-chloro-2'-methoxy[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 119 in file .gra /

RN 592525-98-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-chloro-4'-fluoro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 120 in file .gra /

RN 592526-01-7 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 121 in file .gra /

RN 592526-04-0 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[3'-(trifluoromethoxy){1,1'-biphenyl]-4-yl}methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 122 in file .gra /

RN 592526-07-3 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){(2',6'-dimethoxy[1,1'-biphenyl]-4-yl)methyl}amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 123 in file .gra /

RN 592526-12-0 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4'-(1,1-dimethylethyl){1,1'-biphenyl]-4-yl}methyl}amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 124 in file .gra /

RN 592526-15-3 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[3-[(1,1-dimethylethyl)amino]-3-oxo-1-propen-1-yl]phenyl}methyl}amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 125 in file .gra /

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:304966 CAPLUS <<LOGINID::20080729>>

DOCUMENT NUMBER: 143:2829

TITLE: Molecular Dynamics Simulation of the Ligand Binding Domain of Farnesoid X Receptor. Insights into Helix-12 Stability and Coactivator Peptide Stabilization in Response to Agonist Binding

AUTHOR(S): Costantino, Gabriele; Entrrena-Guadix, Antonio; Macchiarulo, Antonio; Gioiello, Antimo; Pellicciari, Roberto

CORPORATE SOURCE: Dipartimento di Chimica e Tecnologia del Farmaco, Universita di Perugia, Perugia, 06123, Italy

SOURCE: Journal of Medicinal Chemistry (2005), 48(9), 3251-3259

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The dynamic changes which take place in the ligand binding domain (LBD) of farnesoid X receptor (FXR) in response to agonist binding and in the presence of coactivator peptides were studied with nanosecond time-scale mol. dynamics. Four different systems were analyzed, including the holo-LBD complexed with 6ECDCA, the holo-LBD in the presence of two coactivator peptides, and two artificial apo forms, with and without coactivator peptides. Our results revealed a detailed picture of the differential micro- and macromodifications occurring in the LBD in the

presence or not of the agonist mol. and the coactivator peptides. In the apo simulation a major conformational change took place in the crucial helix 12, while the holo-LBD was globally stabilized by the ligand. When the coactivator peptides were included in the simulation, a clear agonist-induced stabilization was obsd. for the canonical peptide. Interestingly, the second peptide was released from the holo-LBD while it was kept bound in the apo simulation. The present results provide a mol. basis for the understanding the role played by the bile acid agonist in receptor stabilization and enhanced cofactor recruitments.

IT        \*\*\*574013-66-4\*\*\* , Fexaramine  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
       (mol. dynamics simulation of ligand binding domain of farnesoid X  
       receptor)  
 RN 574013-66-4 CAPLUS  
 CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4'-(dimethylamino){1,1'-  
      biphenyl]-4-yl}methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 126 in file .gra /

REFERENCE COUNT:        27        THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8        ANSWER 8 OF 13    CAPLUS    COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER:        2004:453343    CAPLUS <>LOGINID::20080729>>  
 DOCUMENT NUMBER:        141:19434  
 TITLE:                    Crystal structure of the human farnesoid X receptor  
                           ligand binding domain complexed with fexaramine and  
                           identification and development of novel small molecule  
                           ligands for FXR  
 INVENTOR(S):            Downes, Michael R.; Verdicia, Mark A.; Noel, Joseph  
                           P.; Evans, Ronald M.; Bowman, Lindsey J.; Bowman,  
                           Marianne  
 PATENT ASSIGNEE(S):     The Salk Institute for Biological Studies, USA  
 SOURCE:                  PCT Int. Appl., 139 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE:          Patent  
 LANGUAGE:                English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004046323	A2	20040603	WO 2003-US36548	20031114
WO 2004046323	A3	20041209		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA,UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003298654	A1	20040615	AU 2003-298654	20031114
US 20060194949	A1	20060831	US 2005-535042	20050513

PRIORITY APPLN. INFO.:

US 2002-426665P P 20021115  
US 2002-426668P P 20021115  
WO 2003-US36548 W 20031114

AB The present invention provides compns. comprising the ligand binding domain (LBD) of a human farnesoid X receptor (FXR) in cryst. form. In alternative embodiments, the LBD of FXR is complexed with a ligand therefor. There are provided high resoln. structures and structure coordinates of FXR complexed with a novel high affinity agonist, fexaramine. The discovered structure of a FXR LBD provides the first three-dimensional view of the structural basis for FXR ligand binding. The present invention further provides a computer for producing a three-dimensional representation of FXR or a complex thereof, and a computer for detg. at least a portion of the structure coordinates of FXR or a complex thereof. The present invention further provides methods of using this structural information to predict mols. capable of binding to FXR; to identify compds. with agonist, antagonist or partial agonist activity for FXR; and to det. whether a test compd. is capable of binding to the LBD of FXR. The present invention further provides compns. comprising compds. identified by such invention methods. Identification and development of novel small mol. ligands for FXR, and activation of FXR and induction of FXR target genes by these novel compds. is disclosed.

IT \*\*\*574013-67-5P\*\*\* , Fexaramine \*\*\*574013-68-6P\*\*\* , Fexarene  
RL: BSU (Biological study, unclassified); CPN (Combinatorial preparation); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)  
(FXR ligand; crystal structure of human farnesoid X receptor ligand binding domain complexed with fexaramine and identification and development of novel small mol. ligands for FXR)

RN 574013-67-5 CAPLUS

CN 2-Propenoic acid, 3-[3-[[4-(1,3-benzodioxol-5-yl)phenyl]methyl](cyclohexylcarbonyl)aminophenyl]-, methyl ester (CA INDEX NAME)

/ Structure 127 in file .gra /

RN 574013-68-6 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(2-phenylethenyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 128 in file .gra /

IT \*\*\*574013-66-4D\*\*\* , Fexaramine, complexes with farnesoid X receptor  
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)  
(crystal structure of human farnesoid X receptor ligand binding domain complexed with fexaramine and identification and development of novel small mol. ligands for FXR)

RN 574013-66-4 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 129 in file .gra /

L8 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:453231 CAPLUS <>LOGINID::20080729>>  
 DOCUMENT NUMBER: 141:23422  
 TITLE: Preparation of non-steroidal FXR agonists  
 INVENTOR(S): Nicolaou, Kyriacos C.; Roecker, Anthony J.; Hughes, Robert; Pfefferkorn, Jeffrey A.  
 PATENT ASSIGNEE(S): The Scripps Research Institute, USA  
 SOURCE: PCT Int. Appl., 75 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004046162	A2	20040603	WO 2003-US36195	20031114
WO 2004046162	A3	20040812		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003290796	A1	20040615	AU 2003-290796	20031114
PRIORITY APPLN. INFO.:			US 2002-426456P	P 20021114
			US 2003-491185P	P 20030729
			WO 2003-US36195	W 20031114
OTHER SOURCE(S):	MARPAT 141:23422			
GI				

/ Structure 130 in file .gra /

AB Non-steroidal N-aryl-N-arylmethyl amido and ureido compds. such as I [E1 = (C1-C8)alkyl, cyclohexyl, 2-furyl, 3-furyl, 2-thienyl, 3-thienyl, Ph, NH(C1-C8)alkyl]; L1, L2 = H; dashed bond = single bond or double bond; X1 = CO, CH2; Y1 = H, NHZ1, NH(2Z)Z3, OZ4; A1 = aryl, heterocyclyl etc.; Z1 = H, Ph, alkyl, benzyl, benzoyl; Z2, Z3 = alkyl; Z2Z3 = cycloalkyl; Z4 = H, oxygen protecting group], were prep'd. for their therapeutic use as farnesoid X receptor (FXR) agonists. Thus, biaryl compd. II, prep'd. via solid phase synthesis starting from N-(tert-butoxycarbonyl)-3-aminocinnamic acid, Merrifield Resin, 4-bromobenzaldehyde, cyclohexanoyl chloride, and 3,4-difluorobenzeneboronic acid, showed FXR activity (EC50 = 72 nM) and relative efficacy = 1.70 at 1-100 mM CDCA from a cell-based assay. The FXR agonists are useful as therapeutic agents for the treatment of diseases linked to cholesterol, bile acids, and their metab. and homeostasis.

IT \*\*\*574013-68-6P\*\*\*  
 RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)

(prepn. of N-aryl-N-arylmethyl amido and ureido compds. as farnesoid X receptor agonists)  
RN 574013-68-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][4-(2-phenylethenyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 131 in file .gra /

IT \*\*\*\*574013-66-4P\*\*\* \*\*\*\*574013-67-5P\*\*\* \*\*\*\*592525-21-8P\*\*\*  
\*\*\*\*592525-23-0P\*\*\* \*\*\*\*592525-29-6P\*\*\* \*\*\*\*592525-32-1P\*\*\*  
\*\*\*\*592525-35-4P\*\*\* \*\*\*\*592525-38-7P\*\*\* \*\*\*\*592525-41-2P\*\*\*  
\*\*\*\*592525-44-5P\*\*\* \*\*\*\*592525-47-8P\*\*\* \*\*\*\*592525-50-3P\*\*\*  
\*\*\*\*592525-55-8P\*\*\* \*\*\*\*592525-58-1P\*\*\* \*\*\*\*592525-61-6P\*\*\*  
\*\*\*\*592525-64-9P\*\*\* \*\*\*\*592525-67-2P\*\*\* \*\*\*\*592525-72-9P\*\*\*  
\*\*\*\*592525-78-5P\*\*\* \*\*\*\*592525-81-0P\*\*\* \*\*\*\*592525-84-3P\*\*\*  
\*\*\*\*592525-87-6P\*\*\* \*\*\*\*592525-90-1P\*\*\* \*\*\*\*592525-93-4P\*\*\*  
\*\*\*\*592525-98-9P\*\*\* \*\*\*\*592526-01-7P\*\*\* \*\*\*\*592526-04-0P\*\*\*  
\*\*\*\*592526-07-3P\*\*\* \*\*\*\*592526-12-0P\*\*\*  
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)  
(prepn. of N-aryl-N-arylmethyl amido and ureido compds. as farnesoid X receptor agonists)  
RN 574013-66-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 132 in file .gra /

RN 574013-67-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[4-(1,3-benzodioxol-5-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 133 in file .gra /

RN 592525-21-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][(3'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 134 in file .gra /

RN 592525-23-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][4'-(methylthio)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 135 in file .gra /

RN 592525-29-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][4-[2-(4-methylphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 136 in file .gra /

RN 592525-32-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2,6-dichlorophenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 137 in file .gra /

RN 592525-35-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[4-[2-(3-chlorophenyl)ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 138 in file .gra /

RN 592525-38-7 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[4-[2-[3,5-bis(trifluoromethyl)phenyl]ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 139 in file .gra /

RN 592525-41-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-[3-(trifluoromethyl)phenyl]ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 140 in file .gra /

RN 592525-44-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2,6-difluorophenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 141 in file .gra /

RN 592525-47-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2-fluorophenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 142 in file .gra /

RN 592525-50-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2,4,6-trimethylphenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 143 in file .gra /

RN 592525-55-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(3-fluorophenyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 144 in file .gra /

RN 592525-58-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(4-fluorophenyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 145 in file .gra /

RN 592525-61-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2-pyridinyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 146 in file .gra /

RN 592525-64-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(4-methyl-5-thiazolyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 147 in file .gra /

RN 592525-67-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){(3',4'-difluoro[1,1'-biphenyl]-4-yl)methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 148 in file .gra /

RN 592525-72-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){(2'-methoxy[1,1'-biphenyl]-4-yl)methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 149 in file .gra /

RN 592525-78-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){(3'-ethoxy[1,1'-biphenyl]-4-yl)methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 150 in file .gra /

RN 592525-81-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){(4'-methoxy[1,1'-biphenyl]-4-

yl)methyl]aminophenyl]-, methyl ester (CA INDEX NAME)

/ Structure 151 in file .gra /

RN 592525-84-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-chloro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)aminophenyl]-, methyl ester (CA INDEX NAME)

/ Structure 152 in file .gra /

RN 592525-87-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 153 in file .gra /

RN 592525-90-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 154 in file .gra /

RN 592525-93-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(5'-chloro-2'-methoxy[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)aminophenyl]-, methyl ester (CA INDEX NAME)

/ Structure 155 in file .gra /

RN 592525-98-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-chloro-4'-fluoro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)aminophenyl]-, methyl ester (CA INDEX NAME)

/ Structure 156 in file .gra /

RN 592526-01-7 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 157 in file .gra /

RN 592526-04-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 158 in file .gra /

RN 592526-07-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2',6'-dimethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 159 in file .gra /

RN 592526-12-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 160 in file .gra /

IT \*\*\*\*592524-75-9P\*\*\*  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. of N-aryl-N-arylmethyl amido and ureido compds. as farnesoid X receptor agonists)  
RN 592524-75-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 161 in file .gra /

IT \*\*\*\*592524-76-0P\*\*\* \*\*\*\*592524-77-1P\*\*\* \*\*\*\*592524-78-2P\*\*\*  
\*\*\*\*592524-79-3P\*\*\* \*\*\*\*592524-80-6P\*\*\* \*\*\*\*592524-81-7P\*\*\*  
\*\*\*\*592524-85-1P\*\*\* \*\*\*\*592524-91-9P\*\*\* \*\*\*\*592524-96-4P\*\*\*  
\*\*\*\*592525-04-7P\*\*\* \*\*\*\*592525-05-8P\*\*\* \*\*\*\*592525-06-9P\*\*\*  
\*\*\*\*592525-07-0P\*\*\* \*\*\*\*592525-08-1P\*\*\* \*\*\*\*592525-09-2P\*\*\*  
\*\*\*\*592525-10-5P\*\*\* \*\*\*\*592525-11-6P\*\*\* \*\*\*\*592525-12-7P\*\*\*  
\*\*\*\*592525-13-8P\*\*\* \*\*\*\*592525-22-9P\*\*\* \*\*\*\*592525-24-1P\*\*\*  
\*\*\*\*592525-25-2P\*\*\* \*\*\*\*592525-27-4P\*\*\* \*\*\*\*592525-28-5P\*\*\*  
\*\*\*\*592526-15-3P\*\*\* \*\*\*\*698360-00-8P\*\*\* \*\*\*\*698363-47-2P\*\*\*  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of N-aryl-N-arylmethyl amido and ureido compds. as farnesoid X receptor agonists)  
RN 592524-76-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl)methyl]amino]phenyl]-, ethyl ester (CA INDEX NAME)

/ Structure 162 in file .gra /

RN 592524-77-1 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 163 in file .gra /

RN 592524-78-2 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(3-(3-amino-3-oxo-1-propen-1-yl)phenyl)(cyclohexylcarbonyl)amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 164 in file .gra /

RN 592524-79-3 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-methoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 165 in file .gra /

RN 592524-80-6 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-ethoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 166 in file .gra /

RN 592524-81-7 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-phenoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 167 in file .gra /

RN 592524-85-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[benzoyl][4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 168 in file .gra /

RN 592524-91-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)(phenylmethyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 169 in file .gra /

RN 592524-96-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 170 in file .gra /

RN 592525-04-7 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 171 in file .gra /

RN 592525-05-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-(3-ethoxy-3-oxo-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 172 in file .gra /

RN 592525-06-9 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1-methylethyl ester (CA INDEX NAME)

/ Structure 173 in file .gra /

RN 592525-07-0 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, phenylmethyl ester (CA INDEX NAME)

/ Structure 174 in file .gra /

RN 592525-08-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[3-(dimethylamino)-3-oxo-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 175 in file .gra /

RN 592525-09-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-(3-methoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 176 in file .gra /

RN 592525-10-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-(3-ethoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 177 in file .gra /

RN 592525-11-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-(3-phenoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 178 in file .gra /

RN 592525-12-7 CAPLUS  
CN Benzenepropanoic acid, 4-[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 179 in file .gra /

RN 592525-13-8 CAPLUS  
CN Benzenepropanoic acid, 4-[(cyclohexylcarbonyl){3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl}amino]methyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 180 in file .gra /

RN 592525-22-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-acetyl[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 181 in file .gra /

RN 592525-24-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(1,1'-biphenyl)-4-ylmethyl](cyclohexylcarbonyl)amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 182 in file .gra /

RN 592525-25-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(5-methyl-2-thienyl)phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 183 in file .gra /

RN 592525-27-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(4-methoxyphenyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 184 in file .gra /

RN 592525-28-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-[4-(1,1-dimethylethyl)phenyl]ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 185 in file .gra /

RN 592526-15-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[3-[(1,1-dimethylethyl)amino]-3-oxo-1-propen-1-yl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 186 in file .gra /

RN 698360-00-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[4-(5-acetyl-2-thienyl)phenyl]methyl]{(2-

methylcyclohexyl)carbonyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 187 in file .gra /

RN 698363-47-2 CAPLUS  
CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]- (CA INDEX NAME)

/ Structure 188 in file .gra /

IT \*\*\*592524-95-3P\*\*\* \*\*\*\*592525-03-6P\*\*\*  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. of N-aryl-N-arylmethyl amido and ureido compds. as farnesoid X  
receptor agonists)  
RN 592524-95-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-bromophenyl)methyl](cyclohexylcarbonyl)amino]p-  
henyl]-, methyl ester (CA INDEX NAME)

/ Structure 189 in file .gra /

RN 592525-03-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[4-(2-carboxyethenyl)phenyl]methyl](cyclohexylcar-  
bonyl)amino]phenyl]-, 1-methyl ester (CA INDEX NAME)

/ Structure 190 in file .gra /

L8 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2004:453152 CAPLUS <>LOGINID::20080729>>  
DOCUMENT NUMBER: 141:17647  
TITLE: N-acyl-N-arylmethylaniline acrylates as nonsteroidal  
farnesoid X receptor modulators  
INVENTOR(S): Downes, Michael R.; Evans, Ronald M.  
PATENT ASSIGNEE(S): The Salk Institute for Biological Studies, USA  
SOURCE: PCT Int. Appl., 98 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004046068	A2	20040603	WO 2003-US36137	20031114
WO 2004046068	A3	20041229		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,			

BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20050143449	A1	20050630	US 2003-658115	20030908
AU 2003294264	A1	20040615	AU 2003-294264	20031114
US 20060128764	A1	20060615	US 2005-535043	20051209
PRIORITY APPLN. INFO.:			US 2002-426664P	P 20021115
			US 2003-658115	A2 20030908
			WO 2003-US36137	W 20031114

OTHER SOURCE(S): MARPAT 141:17647  
GI

/ Structure 191 in file .gra /

AB A method for modulating process(es) mediated by farnesyl X receptor polypeptides comprises conducting said process(es) in the presence of title compd. [I; A = (substituted) alkyl, cycloalkyl, aryl, heteroaryl; X = CO, CH<sub>2</sub>; R = Me, Et; R<sub>1</sub> = H, OH, alkoxy, PhCO<sub>2</sub>, mesityloxy, OCH<sub>2</sub>CO<sub>2</sub>Et; R<sub>2</sub> = H; R<sub>3</sub> = alkenyl, (substituted) aryl, heteroaryl, aralkenyl, heteroaralkenyl; R<sub>2</sub>R<sub>3</sub> = atoms to form a (substituted) (unsatd.) pyran ring; R<sub>4</sub> = H, OH; R<sub>5</sub> = H, OH, alkoxy, aryloxy]. In a cell-based transcription assay, title compd. (II) activated FXR with EC<sub>50</sub> = 36 nM.

IT \*\*\*592524-95-3\*\*\*

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. of N-acyl-N-arylmethylaniline acrylates as nonsteroidal farnesoid X receptor modulators)

RN 592524-95-3 CAPLUS

CN 2-Propenoic acid, 3-[3-[(4-bromophenyl)methyl](cyclohexylcarbonyl)amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 192 in file .gra /

IT ***574013-66-4P***	****574013-67-5P***	****574013-68-6P***
***592524-75-9P***	****592524-76-0P***	****592524-77-1P***
***592524-78-2P***	****592524-79-3P***	***592524-80-6P***
***592524-81-7P***	****592524-85-1P***	****592524-91-9P***
***592524-96-4P***	****592525-03-6P***	****592525-04-7P***
***592525-05-8P***	****592525-06-9P***	***592525-07-0P***
***592525-08-1P***	****592525-09-2P***	****592525-10-5P***
***592525-11-6P***	****592525-12-7P***	****592525-13-8P***
***592525-21-8P***	****592525-22-9P***	***592525-23-0P***
***592525-24-1P***	****592525-25-2P***	****592525-26-3P***
***592525-27-4P***	****592525-28-5P***	****592525-29-6P***
***592525-32-1P***	****592525-35-4P***	***592525-38-7P***
***592525-41-2P***	****592525-44-5P***	****592525-47-8P***
***592525-50-3P***	****592525-55-8P***	****592525-58-1P***
***592525-61-6P***	****592525-64-9P***	***592525-67-2P***
***592525-72-9P***	****592525-78-5P***	***592525-81-0P***
***592525-84-3P***	****592525-87-6P***	***592525-90-1P***
***592525-93-4P***	****592525-98-9P***	***592526-01-7P***

\*\*\*592526-04-0P\*\*\*      \*\*\*592526-07-3P\*\*\*      \*\*\*592526-12-0P\*\*\*  
\*\*\*592526-16-4P\*\*\*      \*\*\*699006-40-1P\*\*\*      \*\*\*699006-41-2P\*\*\*  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)  
    (prepn. of N-acyl-N-arylmethylaniline acrylates as nonsteroidal  
    farnesoid X receptor modulators)  
RN 574013-66-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4'-(dimethylamino)[1,1'-  
biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)  
  
/ Structure 193 in file .gra /  
  
RN 574013-67-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-(1,3-benzodioxol-5-  
yl)phenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA  
INDEX NAME)  
  
/ Structure 194 in file .gra /  
  
RN 574013-68-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4-(2-  
phenylethenyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)  
  
/ Structure 195 in file .gra /  
  
RN 592524-75-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4-[3-(1,1-dimethylethoxy)-3-  
oxo-1-propen-1-yl]phenyl}methyl]amino]phenyl]-, methyl ester (CA INDEX  
NAME)  
  
/ Structure 196 in file .gra /  
  
RN 592524-76-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4-[3-(1,1-dimethylethoxy)-3-  
oxo-1-propen-1-yl]phenyl}methyl]amino]phenyl]-, ethyl ester (CA INDEX  
NAME)  
  
/ Structure 197 in file .gra /  
  
RN 592524-77-1 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[{3-[3-(1,1-dimethylethoxy)-3-  
oxo-1-propen-1-yl]phenyl}methyl]amino]phenyl]-, 1,1-dimethylethyl ester  
(CA INDEX NAME)  
  
/ Structure 198 in file .gra /  
  
RN 592524-78-2 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(3-(3-amino-3-oxo-1-propen-1-  
yl)phenyl)(cyclohexylcarbonyl)amino]methyl]phenyl]-, 1,1-dimethylethyl  
ester (CA INDEX NAME)

/ Structure 199 in file .gra /

RN 592524-79-3 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){3-(3-methoxy-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 200 in file .gra /

RN 592524-80-6 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){3-(3-ethoxy-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 201 in file .gra /

RN 592524-81-7 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){3-(3-phenoxy-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 202 in file .gra /

RN 592524-85-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[benzoyl][4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 203 in file .gra /

RN 592524-91-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)(phenylmethyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 204 in file .gra /

RN 592524-96-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(1,1-dimethylethyl)phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 205 in file .gra /

RN 592525-03-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-(2-carboxyethenyl)phenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, 1-methyl ester (CA INDEX NAME)

/ Structure 206 in file .gra /

RN 592525-04-7 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 207 in file .gra /

RN 592525-05-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-(3-ethoxy-3-oxo-1-propen-1-yl)phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 208 in file .gra /

RN 592525-06-9 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1-methylethyl ester (CA INDEX NAME)

/ Structure 209 in file .gra /

RN 592525-07-0 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, phenylmethyl ester (CA INDEX NAME)

/ Structure 210 in file .gra /

RN 592525-08-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[3-(dimethylamino)-3-oxo-1-propen-1-yl)phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 211 in file .gra /

RN 592525-09-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-(3-methoxy-1-propen-1-yl)phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 212 in file .gra /

RN 592525-10-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-(3-ethoxy-1-propen-1-yl)phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 213 in file .gra /

RN 592525-11-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-(3-phenoxy-1-propen-1-yl)phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 214 in file .gra /

RN 592525-12-7 CAPLUS  
CN Benzenepropanoic acid, 4-[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 215 in file .gra /

RN 592525-13-8 CAPLUS  
CN Benzenepropanoic acid, 4-[(cyclohexylcarbonyl){3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl}amino]methyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 216 in file .gra /

RN 592525-21-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){(3'-methoxy[1,1'-biphenyl]-4-yl)methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 217 in file .gra /

RN 592525-22-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-acetyl[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 218 in file .gra /

RN 592525-23-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4'-(methylthio)[1,1'-biphenyl]-4-yl)methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 219 in file .gra /

RN 592525-24-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(1,1'-biphenyl)-4-ylmethyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 220 in file .gra /

RN 592525-25-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(5-methyl-2-thienyl)phenyl)methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 221 in file .gra /

RN 592525-26-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-(5-acetyl-2-thienyl)phenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 222 in file .gra /

RN 592525-27-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(4-methoxyphenyl)ethenyl]phenyl)methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

INDEX NAME)

/ Structure 223 in file .gra /

RN 592525-28-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-[4-(1,1-dimethylethyl)phenyl]ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester  
(CA INDEX NAME)

/ Structure 224 in file .gra /

RN 592525-29-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(4-methylphenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 225 in file .gra /

RN 592525-32-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2,6-dichlorophenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 226 in file .gra /

RN 592525-35-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[[4-[2-(3-chlorophenyl)ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 227 in file .gra /

RN 592525-38-7 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[[4-[2-[3,5-bis(trifluoromethyl)phenyl]ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 228 in file .gra /

RN 592525-41-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-[3-(trifluoromethyl)phenyl]ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester  
(CA INDEX NAME)

/ Structure 229 in file .gra /

RN 592525-44-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2,6-difluorophenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 230 in file .gra /

RN 592525-47-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2-fluorophenyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 231 in file .gra /

RN 592525-50-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2,4,6-trimethylphenyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 232 in file .gra /

RN 592525-55-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(3-fluorophenyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 233 in file .gra /

RN 592525-58-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(4-fluorophenyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 234 in file .gra /

RN 592525-61-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2-pyridinyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 235 in file .gra /

RN 592525-64-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(4-methyl-5-thiazolyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 236 in file .gra /

RN 592525-67-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){(3',4'-difluoro[1,1'-biphenyl]-4-yl)methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 237 in file .gra /

RN 592525-72-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)|(2'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 238 in file .gra /

RN 592525-78-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)|(3'-ethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 239 in file .gra /

RN 592525-81-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)|(4'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 240 in file .gra /

RN 592525-84-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-chloro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 241 in file .gra /

RN 592525-87-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)|(4'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 242 in file .gra /

RN 592525-90-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)|(3'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 243 in file .gra /

RN 592525-93-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(5'-chloro-2'-methoxy[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 244 in file .gra /

RN 592525-98-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-chloro-4'-fluoro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 245 in file .gra /

RN 592526-01-7 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 246 in file .gra /

RN 592526-04-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 247 in file .gra /

RN 592526-07-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[2',6'-dimethoxy[1,1'-biphenyl]-4-yl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 248 in file .gra /

RN 592526-12-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 249 in file .gra /

RN 592526-16-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[3',5'-dichloro[1,1'-biphenyl]-4-yl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 250 in file .gra /

RN 699006-40-1 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, 2-methylpropyl ester (CA INDEX NAME)

/ Structure 251 in file .gra /

RN 699006-41-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[3-[(2-methylpropyl)amino]-3-oxo-1-propen-1-yl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 252 in file .gra /

L8 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2004:452954 CAPLUS <>LOGINID::20080729>>  
DOCUMENT NUMBER: 141:17646

TITLE: N-acyl-N-benzylaniline acrylates as nonsteroidal  
 farnesoid X receptor (FXR) modulators  
 INVENTOR(S): Downes, Michael R.; Evans, Ronald Mark; Hughes,  
 Robert; Nicolaou, Kyriacos C.; Roecker, Anthony J.  
 PATENT ASSIGNEE(S): The Salk Institute for Biological Studies, USA; The  
 Scripps Research Institute  
 SOURCE: PCT Int. Appl., 62 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004045511	A2	20040603	WO 2003-US36123	20031114
WO 2004045511	A3	20040708		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20050143449	A1	20050630	US 2003-658115	20030908
AU 2003290778	A1	20040615	AU 2003-290778	20031114
US 20060223879	A1	20061005	US 2005-535041	20051228
PRIORITY APPLN. INFO.:			US 2002-426664P	P 20021115
			US 2003-658115	A2 20030908
			WO 2003-US36123	W 20031114

OTHER SOURCE(S): MARPAT 141:17646  
 GI

/ Structure 253 in file .gra /

AB Title compds. [I; A = (substituted) alkyl, cycloalkyl, aryl, heteroaryl; X = CO, CH2; R = Me, Et; R1 = H, OH, alkoxy, PhCO2, mesityloxy, OCH2CO2Et; R2 = H; R3 = alkenyl, (substituted) aryl, heteroaryl, aralkenyl, heteroaralkenyl; R2R3 = atoms to form a substituted (unsatd.) pyran ring; R4 = H, OH; R5 = H, OH, alkoxy, aryloxy], are claimed. Thus, benzopyran deriv. (II) activated FXR receptors with EC50 = 358 nM.

IT \*\*\*592524-95-3P\*\*\*

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (prepn. of acylbenzylaniline acrylates as nonsteroidal farnesoid X receptor (FXR) modulators)

RN 592524-95-3 CAPLUS

CN 2-Propenoic acid, 3-[3-[(4-bromophenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 254 in file .gra /

IT      \*\*\*\*574013-66-4P\*\*\*      \*\*\*\*574013-67-5P\*\*\*      \*\*\*\*574013-68-6P\*\*\*  
\*\*\*\*592524-75-9P\*\*\*      \*\*\*\*592524-76-0P\*\*\*      \*\*\*\*592524-77-1P\*\*\*  
\*\*\*\*592524-78-2P\*\*\*      \*\*\*\*592524-79-3P\*\*\*      \*\*\*\*592524-80-6P\*\*\*  
\*\*\*\*592524-81-7P\*\*\*      \*\*\*\*592524-85-1P\*\*\*      \*\*\*\*592524-91-9P\*\*\*  
\*\*\*\*592524-96-4P\*\*\*      \*\*\*\*592525-03-6P\*\*\*      \*\*\*\*592525-04-7P\*\*\*  
\*\*\*\*592525-05-8P\*\*\*      \*\*\*\*592525-06-9P\*\*\*      \*\*\*\*592525-07-0P\*\*\*  
\*\*\*\*592525-08-1P\*\*\*      \*\*\*\*592525-09-2P\*\*\*      \*\*\*\*592525-10-5P\*\*\*  
\*\*\*\*592525-11-6P\*\*\*      \*\*\*\*592525-12-7P\*\*\*      \*\*\*\*592525-21-8P\*\*\*  
\*\*\*\*592525-22-9P\*\*\*      \*\*\*\*592525-23-0P\*\*\*      \*\*\*\*592525-24-1P\*\*\*  
\*\*\*\*592525-25-2P\*\*\*      \*\*\*\*592525-26-3P\*\*\*      \*\*\*\*592525-27-4P\*\*\*  
\*\*\*\*592525-28-5P\*\*\*      \*\*\*\*592525-29-6P\*\*\*      \*\*\*\*592525-32-1P\*\*\*  
\*\*\*\*592525-35-4P\*\*\*      \*\*\*\*592525-38-7P\*\*\*      \*\*\*\*592525-41-2P\*\*\*  
\*\*\*\*592525-44-5P\*\*\*      \*\*\*\*592525-47-8P\*\*\*      \*\*\*\*592525-50-3P\*\*\*  
\*\*\*\*592525-55-8P\*\*\*      \*\*\*\*592525-58-1P\*\*\*      \*\*\*\*592525-61-6P\*\*\*  
\*\*\*\*592525-64-9P\*\*\*      \*\*\*\*592525-67-2P\*\*\*      \*\*\*\*592525-72-9P\*\*\*  
\*\*\*\*592525-78-5P\*\*\*      \*\*\*\*592525-81-0P\*\*\*      \*\*\*\*592525-84-3P\*\*\*  
\*\*\*\*592525-87-6P\*\*\*      \*\*\*\*592525-90-1P\*\*\*      \*\*\*\*592525-93-4P\*\*\*  
\*\*\*\*592525-98-9P\*\*\*      \*\*\*\*592526-01-7P\*\*\*      \*\*\*\*592526-04-0P\*\*\*  
\*\*\*\*592526-07-3P\*\*\*      \*\*\*\*592526-12-0P\*\*\*      \*\*\*\*592526-15-3P\*\*\*  
\*\*\*\*592526-16-4P\*\*\*      \*\*\*\*699021-26-6P\*\*\*

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of acylbenzylaniline acrylates as nonsteroidal farnesoid X receptor (FXR) modulators)

RN 574013-66-4 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 255 in file .gra /

RN 574013-67-5 CAPLUS

CN 2-Propenoic acid, 3-[3-[(4-(1,3-benzodioxol-5-yl)phenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 256 in file .gra /

RN 574013-68-6 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(2-phenylethyl)phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 257 in file .gra /

RN 592524-75-9 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 258 in file .gra /

RN 592524-76-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl}amino]phenyl]-, ethyl ester (CA INDEX NAME)

/ Structure 259 in file .gra /

RN 592524-77-1 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl}amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 260 in file .gra /

RN 592524-78-2 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(3-amino-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 261 in file .gra /

RN 592524-79-3 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){3-(3-methoxy-1-propen-1-yl)phenyl}amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 262 in file .gra /

RN 592524-80-6 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){3-(3-ethoxy-1-propen-1-yl)phenyl}amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 263 in file .gra /

RN 592524-81-7 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){3-(3-phenoxy-1-propen-1-yl)phenyl}amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 264 in file .gra /

RN 592524-85-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[benzoyl]{[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 265 in file .gra /

RN 592524-91-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)(phenylmethyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 266 in file .gra /

RN 592524-96-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(1,1-dimethylethyl)phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 267 in file .gra /

RN 592525-03-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[4-(2-carboxyethenyl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, 1-methyl ester (CA INDEX NAME)

/ Structure 268 in file .gra /

RN 592525-04-7 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 269 in file .gra /

RN 592525-05-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(3-ethoxy-3-oxo-1-propen-1-yl)phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 270 in file .gra /

RN 592525-06-9 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, 1-methylethyl ester (CA INDEX NAME)

/ Structure 271 in file .gra /

RN 592525-07-0 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, phenylmethyl ester (CA INDEX NAME)

/ Structure 272 in file .gra /

RN 592525-08-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[3-(dimethylamino)-3-oxo-1-propen-1-yl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 273 in file .gra /

RN 592525-09-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(3-methoxy-1-propen-1-yl)phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 274 in file .gra /

RN 592525-10-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4-(3-ethoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 275 in file .gra /

RN 592525-11-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4-(3-phenoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 276 in file .gra /

RN 592525-12-7 CAPLUS  
CN Benzenepropanoic acid, 4-[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 277 in file .gra /

RN 592525-21-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{(3'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 278 in file .gra /

RN 592525-22-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-acetyl[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 279 in file .gra /

RN 592525-23-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4'-(methylthio)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 280 in file .gra /

RN 592525-24-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(1,1'-biphenyl)-4-ylmethyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 281 in file .gra /

RN 592525-25-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4-(5-methyl-2-thienyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 282 in file .gra /

RN 592525-26-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-(5-acetyl-2-thienyl)phenyl)methyl](cyclohexylcarbonyl)amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 283 in file .gra /

RN 592525-27-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(4-methoxyphenyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 284 in file .gra /

RN 592525-28-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(4-(1,1-dimethylethyl)phenyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 285 in file .gra /

RN 592525-29-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(4-methylphenyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 286 in file .gra /

RN 592525-32-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(2,6-dichlorophenyl)ethenyl]phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 287 in file .gra /

RN 592525-35-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-[2-(3-chlorophenyl)ethenyl]phenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 288 in file .gra /

RN 592525-38-7 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-[2-(3,5-bis(trifluoromethyl)phenyl)ethenyl]phenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 289 in file .gra /

RN 592525-41-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-[3-(trifluoromethyl)phenyl]ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 290 in file .gra /

RN 592525-44-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2,6-difluorophenyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 291 in file .gra /

RN 592525-47-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2-fluorophenyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 292 in file .gra /

RN 592525-50-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2,4,6-trimethylphenyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 293 in file .gra /

RN 592525-55-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(3-fluorophenyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 294 in file .gra /

RN 592525-58-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(4-fluorophenyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 295 in file .gra /

RN 592525-61-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2-pyridinyl)ethenyl]phenyl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 296 in file .gra /

RN 592525-64-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[4-[2-(4-methyl-5-thiazolyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 297 in file .gra /

RN 592525-67-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',4'-difluoro[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 298 in file .gra /

RN 592525-72-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 299 in file .gra /

RN 592525-78-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-ethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 300 in file .gra /

RN 592525-81-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 301 in file .gra /

RN 592525-84-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-chloro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 302 in file .gra /

RN 592525-87-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 303 in file .gra /

RN 592525-90-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 304 in file .gra /

RN 592525-93-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(5'-chloro-2'-methoxy[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 305 in file .gra /

RN 592525-98-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-chloro-4'-fluoro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 306 in file .gra /

RN 592526-01-7 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl)methyl]amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 307 in file .gra /

RN 592526-04-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl)methyl]amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 308 in file .gra /

RN 592526-07-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2',6'-dimethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 309 in file .gra /

RN 592526-12-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl)methyl]amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 310 in file .gra /

RN 592526-15-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[4-[3-[(1,1-dimethylethyl)amino]-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 311 in file .gra /

RN 592526-16-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',5'-dichloro[1,1'-biphenyl]-4-yl)methyl]amino]phenyl-, methyl ester (CA INDEX NAME)

/ Structure 312 in file .gra /

RN 699021-26-6 CAPLUS  
CN Benzenepropanoic acid, 4-[(cyclohexylcarbonyl){3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino}methyl]-, methyl ester (CA INDEX NAME)

/ Structure 313 in file .gra /

L8 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2003:375244 CAPLUS <>LOGINID:20080729>>  
DOCUMENT NUMBER: 139:159454  
TITLE: A chemical, genetic, and structural analysis of the  
nuclear bile acid receptor FXR  
AUTHOR(S): Downes, Michael; Verdecia, Mark A.; Roecker, A. J.;  
Hughes, Robert; Hogenesch, John B.; Kast-Woelbern,  
Heidi R.; Bowman, Marianne E.; Ferrer, Jean-Luc;  
Anisfeld, Andrew M.; Edwards, Peter A.; Rosenfeld,  
John M.; Alvarez, Jacqueline G. A.; Noel, Joseph P.;  
Nicolaou, K. C.; Evans, Ronald M.  
CORPORATE SOURCE: Gene Expression Laboratory, Howard Hughes Medical  
Institute, La Jolla, CA, 92037, USA  
SOURCE: Molecular Cell (2003), 11(4), 1079-1092  
CODEN: MOCEFL; ISSN: 1097-2765  
PUBLISHER: Cell Press  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The farnesoid X receptor (FXR) functions as a bile acid (BA) sensor  
coordinating cholesterol metab., lipid homeostasis, and absorption of  
dietary fats and vitamins. However, BAs are poor reagents for  
characterizing FXR functions due to multiple receptor independent  
properties. Accordingly, using combinatorial chem. we evolved a small  
mol. agonist termed fexaramine with 100-fold increased affinity relative  
to natural compds. Gene-profiling expts. conducted in hepatocytes with  
FXR-specific fexaramine vs. the primary BA chenodeoxycholic acid (CDCA)  
produced remarkably distinct genomic targets. Highly diffracting  
cocrystals (1.78 .ANG.) of fexaramine bound to the ligand binding domain  
of FXR revealed the agonist sequestered in a 726 .ANG.3 hydrophobic cavity  
and suggest a mechanistic basis for the initial step in the BA signaling  
pathway. The discovery of fexaramine will allow us to unravel the FXR  
genetic network from the BA network and selectively manipulate components  
of the cholesterol pathway that may be useful in treating  
cholesterol-related human diseases.  
IT \*\*\*574013-66-4P\*\*\* , Fexaramine \*\*\*574013-67-5P\*\*\* , Fexarine  
\*\*\*574013-68-6P\*\*\* , Fexarene  
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PRP  
(Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL  
(Biological study); PREP (Preparation); USES (Uses)  
(chem., genetic, and structural anal. of nuclear bile acid receptor  
FXR)  
RN 574013-66-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4'-(dimethylamino)[1,1'-  
biphenyl]-4-yl]methyl}amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 314 in file .gra /

RN 574013-67-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-(1,3-benzodioxol-5-yl)phenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 315 in file .gra /

RN 574013-68-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)(4-(2-phenylethenyl)phenyl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 316 in file .gra /

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2003:354702 CAPLUS <>LOGINID::20080729>>  
DOCUMENT NUMBER: 139:224366  
TITLE: Discovery and optimization of non-steroidal FXR  
agonists from natural product-like libraries  
AUTHOR(S): Nicolaou, K. C.; Evans, Ronald M.; Roecker, A. J.;  
Hughes, Robert; Downes, Michael; Pfefferkorn, Jeffery  
A.  
CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for  
Chemical Biology, The Scripps Research Institute, La  
Jolla, CA, 92037, USA  
SOURCE: Organic & Biomolecular Chemistry (2003), 1(6), 908-920  
CODEN: OBCRAK; ISSN: 1477-0520  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The efficient regulation of cholesterol biosynthesis, metab., acquisition, and transport is an essential component of lipid homeostasis. The farnesoid X receptor (FXR) is a transcriptional sensor for bile acids, the primary product of cholesterol metab. Accordingly, the development of potent, selective, small mol. agonists, partial agonists, and antagonists of FXR would be an important step in further deconvoluting FXR physiol. Herein, we describe the development of four novel classes of potent FXR activators originating from natural product-like libraries. Initial screening of a 10000-membered, diversity-orientated library of benzopyran contg. small mols. for FXR activation utilizing a cell-based reporter assay led to the identification of several lead compds. possessing low micromolar activity (EC50's = 5-10 .mu.M). These compds. were systematically optimized employing parallel soln.-phase synthesis and solid-phase synthesis to provide four classes of compds. that potently activate FXR. Two series of compds., bearing stilbene or biaryl moieties, contain members that are the most potent FXR agonists reported to date in cell-based assays. These compds. may find future utility as chem. tools in studies aimed at further defining the physiol. role of FXR and discovering potential therapeutic agents for the treatment of diseases linked to cholesterol and bile acid metab. and homeostasis.

IT \*\*\*574013-66-4\*\*\* \*\*\*574013-67-5\*\*\* \*\*\*574013-68-6\*\*\*

\*\*\*\*592524-75-9\*\*\*\* \*\*\*\*592524-76-0\*\*\*\* \*\*\*\*592524-77-1\*\*\*\*  
\*\*\*\*592524-78-2\*\*\*\* \*\*\*\*592524-79-3\*\*\*\* \*\*\*\*592524-80-6\*\*\*\*  
\*\*\*\*592524-81-7\*\*\*\* \*\*\*\*592524-85-1\*\*\*\* \*\*\*\*592524-91-9\*\*\*\*  
\*\*\*\*592524-95-3\*\*\*\* \*\*\*\*592524-96-4\*\*\*\* \*\*\*\*592525-03-6\*\*\*\*  
\*\*\*\*592525-04-7\*\*\*\* \*\*\*\*592525-05-8\*\*\*\* \*\*\*\*592525-06-9\*\*\*\*  
\*\*\*\*592525-07-0\*\*\*\* \*\*\*\*592525-08-1\*\*\*\* \*\*\*\*592525-09-2\*\*\*\*  
\*\*\*\*592525-10-5\*\*\*\* \*\*\*\*592525-11-6\*\*\*\* \*\*\*\*592525-12-7\*\*\*\*  
\*\*\*\*592525-13-8\*\*\*\* \*\*\*\*592525-21-8\*\*\*\* \*\*\*\*592525-22-9\*\*\*\*  
\*\*\*\*592525-23-0\*\*\*\* \*\*\*\*592525-24-1\*\*\*\* \*\*\*\*592525-25-2\*\*\*\*  
\*\*\*\*592525-26-3\*\*\*\* \*\*\*\*592525-27-4\*\*\*\* \*\*\*\*592525-28-5\*\*\*\*  
\*\*\*\*592525-29-6\*\*\*\* \*\*\*\*592525-32-1\*\*\*\* \*\*\*\*592525-35-4\*\*\*\*  
\*\*\*\*592525-38-7\*\*\*\* \*\*\*\*592525-41-2\*\*\*\* \*\*\*\*592525-44-5\*\*\*\*  
\*\*\*\*592525-47-8\*\*\*\* \*\*\*\*592525-50-3\*\*\*\* \*\*\*\*592525-55-8\*\*\*\*  
\*\*\*\*592525-58-1\*\*\*\* \*\*\*\*592525-61-6\*\*\*\* \*\*\*\*592525-64-9\*\*\*\*  
\*\*\*\*592525-67-2\*\*\*\* \*\*\*\*592525-72-9\*\*\*\* \*\*\*\*592525-78-5\*\*\*\*  
\*\*\*\*592525-81-0\*\*\*\* \*\*\*\*592525-84-3\*\*\*\* \*\*\*\*592525-87-6\*\*\*\*  
\*\*\*\*592525-90-1\*\*\*\* \*\*\*\*592525-93-4\*\*\*\* \*\*\*\*592525-98-9\*\*\*\*  
\*\*\*\*592526-01-7\*\*\*\* \*\*\*\*592526-04-0\*\*\*\* \*\*\*\*592526-07-3\*\*\*\*  
\*\*\*\*592526-12-0\*\*\*\* \*\*\*\*592526-15-3\*\*\*\* \*\*\*\*592526-16-4\*\*\*\*

RL: PAC (Pharmacological activity); BIOL (Biological study)  
(discovery and optimization of non-steroidal FXR agonists from natural  
product-like libraries)

RN 574013-66-4 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 317 in file .gra /

RN 574013-67-5 CAPLUS

CN 2-Propenoic acid, 3-[3-[[4-(1,3-benzodioxol-5-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 318 in file .gra /

RN 574013-68-6 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][4-(2-phenylethenyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 319 in file .gra /

RN 592524-75-9 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 320 in file .gra /

RN 592524-76-0 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)][4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, ethyl ester (CA INDEX NAME)

/ Structure 321 in file .gra /

RN 592524-77-1 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester  
(CA INDEX NAME)

/ Structure 322 in file .gra /

RN 592524-78-2 CAPLUS  
CN 2-Propenoic acid, 3-[4-[[3-(3-amino-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]phenyl]-, 1,1-dimethylethyl ester  
(CA INDEX NAME)

/ Structure 323 in file .gra /

RN 592524-79-3 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-methoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester  
(CA INDEX NAME)

/ Structure 324 in file .gra /

RN 592524-80-6 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-ethoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester  
(CA INDEX NAME)

/ Structure 325 in file .gra /

RN 592524-81-7 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl)[3-(3-phenoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester  
(CA INDEX NAME)

/ Structure 326 in file .gra /

RN 592524-85-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[benzoyl][4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]phenyl]-, methyl ester  
(CA INDEX NAME)

/ Structure 327 in file .gra /

RN 592524-91-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)(phenylmethyl)amino]phenyl]-, methyl ester  
(CA INDEX NAME)

/ Structure 328 in file .gra /

RN 592524-95-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-bromophenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester  
(CA INDEX NAME)

/ Structure 329 in file .gra /

RN 592524-96-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(1,1-dimethylethyl)phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 330 in file .gra /

RN 592525-03-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[4-(2-carboxyethenyl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, 1-methyl ester (CA INDEX NAME)

/ Structure 331 in file .gra /

RN 592525-04-7 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 332 in file .gra /

RN 592525-05-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(3-ethoxy-3-oxo-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 333 in file .gra /

RN 592525-06-9 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, 1-methylethyl ester (CA INDEX NAME)

/ Structure 334 in file .gra /

RN 592525-07-0 CAPLUS  
CN 2-Propenoic acid, 3-[4-[(cyclohexylcarbonyl){[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino}methyl]phenyl]-, phenylmethyl ester (CA INDEX NAME)

/ Structure 335 in file .gra /

RN 592525-08-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[3-(dimethylamino)-3-oxo-1-propen-1-yl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 336 in file .gra /

RN 592525-09-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(3-methoxy-1-propen-1-yl)phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 337 in file .gra /

RN 592525-10-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4-(3-ethoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 338 in file .gra /

RN 592525-11-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4-(3-phenoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 339 in file .gra /

RN 592525-12-7 CAPLUS  
CN Benzenepropanoic acid, 4-[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 340 in file .gra /

RN 592525-13-8 CAPLUS  
CN Benzenepropanoic acid, 4-[(cyclohexylcarbonyl)[3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 341 in file .gra /

RN 592525-21-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{(3'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 342 in file .gra /

RN 592525-22-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-acetyl[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 343 in file .gra /

RN 592525-23-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4'-(methylthio)[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 344 in file .gra /

RN 592525-24-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(1,1'-biphenyl)-4-ylmethyl](cyclohexylcarbonyl)am

inolphenyl]-, methyl ester (CA INDEX NAME)

/ Structure 345 in file .gra /

RN 592525-25-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-(5-methyl-2-thienyl)phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 346 in file .gra /

RN 592525-26-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[[4-(5-acetyl-2-thienyl)phenyl]methyl](cyclohexylcarbonyl)amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 347 in file .gra /

RN 592525-27-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(4-methoxyphenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 348 in file .gra /

RN 592525-28-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-[4-(1,1-dimethylethyl)phenyl]ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 349 in file .gra /

RN 592525-29-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(4-methylphenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 350 in file .gra /

RN 592525-32-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl){[4-[2-(2,6-dichlorophenyl)ethenyl]phenyl]methyl]amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 351 in file .gra /

RN 592525-35-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[[[4-[2-(3-chlorophenyl)ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino}phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 352 in file .gra /

RN 592525-38-7 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(4-[2-[3,5-bis(trifluoromethyl)phenyl]ethenyl]phenyl)methyl](cyclohexylcarbonyl)aminophenyl]-, methyl ester (CA INDEX NAME)

/ Structure 353 in file .gra /

RN 592525-41-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-[3-trifluoromethyl]phenyl]ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 354 in file .gra /

RN 592525-44-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(2,6-difluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 355 in file .gra /

RN 592525-47-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(2-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 356 in file .gra /

RN 592525-50-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(2,4,6-trimethylphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 357 in file .gra /

RN 592525-55-8 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(3-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 358 in file .gra /

RN 592525-58-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4-[2-(4-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 359 in file .gra /

RN 592525-61-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2-pyridinyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 360 in file .gra /

RN 592525-64-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methyl-5-thiazolyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 361 in file .gra /

RN 592525-67-2 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',4'-difluoro[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 362 in file .gra /

RN 592525-72-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 363 in file .gra /

RN 592525-78-5 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-ethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 364 in file .gra /

RN 592525-81-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 365 in file .gra /

RN 592525-84-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-chloro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 366 in file .gra /

RN 592525-87-6 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 367 in file .gra /

RN 592525-90-1 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 368 in file .gra /

RN 592525-93-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(5'-chloro-2'-methoxy[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 369 in file .gra /

RN 592525-98-9 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(3'-chloro-4'-fluoro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 370 in file .gra /

RN 592526-01-7 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl}methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 371 in file .gra /

RN 592526-04-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl}methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 372 in file .gra /

RN 592526-07-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{(2',6'-dimethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 373 in file .gra /

RN 592526-12-0 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl}methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 374 in file .gra /

RN 592526-15-3 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[{4-[3-[(1,1-dimethylethyl)amino]-3-oxo-1-propen-1-yl]phenyl}methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 375 in file .gra /

RN 592526-16-4 CAPLUS  
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)((3',5'-dichloro[1,1'-biphenyl]-4-yl)methyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 376 in file .gra /

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1.80 441.83

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